Appendix D. Matrix decompositions for mass matrix diagonalization

In scalar field theory, the diagonalization of the scalar squared-mass matrix M^2 is straightforward. For a theory of n complex scalar fields, M^2 is an hermitian $n \times n$ matrix, which can be diagonalized by a unitary matrix W:

$$W^\dagger M^2 W = m^2 = \text{diag}(m_1^2, m_2^2, \ldots, m_n^2). \tag{D.1}$$

For a theory of n real scalar fields, M^2 is a real symmetric $n \times n$ matrix, which can be diagonalized by an orthogonal matrix Q:

$$Q^{\mathsf{T}} M^2 Q = m^2 = \text{diag}(m_1^2, m_2^2, \ldots, m_n^2). \tag{D.2}$$

In both cases, the eigenvalues m_k^2 of M^2 are real. These are the standard matrix diagonalization problems that are treated in all elementary linear algebra textbooks.

In spin-1/2 fermion field theory, the most general fermion mass matrix, obtained from the Lagrangian, written in terms of two-component spinors, is complex and symmetric [cf. Section 3.2]. If the Lagrangian exhibits a U(1) symmetry, then a basis can be found such that fields that are charged under the U(1) pair up into Dirac fermions. The fermion mass matrix then decomposes into the direct sum of a complex Dirac fermion mass matrix and a complex symmetric neutral fermion mass matrix. In this Appendix, we review the linear algebra theory relevant for the matrix decompositions associated with the general charged and neutral spin-1/2 fermion mass matrix diagonalizations. The diagonalization of the Dirac fermion mass matrix is governed by the singular value decomposition of a complex matrix, as shown in Appendix D.1. In contrast, the diagonalization of a neutral fermion mass matrix is governed by the Takagi diagonalization of a complex symmetric matrix, which is treated in Appendix D.2.[99] These two techniques are compared and contrasted in Appendix D.3. Dirac fermions can also arise in the case of a pseudo-real representation of fermion fields. As shown in Section 3.2, this latter case requires the reduction of a complex antisymmetric fermion mass matrix to real normal form. The relevant theorem and its proof are given in Appendix D.4.

D.1. Singular value decomposition

The diagonalization of the charged (Dirac) fermion mass matrix requires the singular value decomposition of an arbitrary complex matrix M.

Theorem. *For any complex [or real] $n \times n$ matrix M, unitary [or real orthogonal] matrices L and R exist such that*

$$L^{\mathsf{T}} M R = M_D = \text{diag}(m_1, m_2, \ldots, m_n), \tag{D.1.1}$$

where the m_k are real and non-negative. This is called the singular value decomposition of the matrix M (e.g., see Refs. [147,258]).

In general, the m_k are *not* the eigenvalues of M. Rather, the m_k are the *singular values* of the general complex matrix M, which are defined to be the non-negative square roots of the eigenvalues of $M^\dagger M$ (or equivalently of $MM^\dagger$). An equivalent definition of the singular values can be established as follows. Since $M^\dagger M$ is an hermitian non-negative matrix, its eigenvalues are real and non-negative and its eigenvectors, v_k, defined by $M^\dagger M v_k = m_k^2 v_k$, can be chosen to be orthonormal.[100] Consider first the eigenvectors corresponding to the non-zero eigenvalues of $M^\dagger M$. Then, we define the vectors w_k such that $M v_k = m_k w_k^*$. It follows that $m_k^2 v_k = M^\dagger M v_k = m_k M^\dagger w_k^*$, which yields: $M^\dagger w_k^* = m_k v_k$. Note that these equations also imply that $MM^\dagger w_k^* = m_k^2 w_k^*$. The orthonormality of the v_k implies the orthonormality of the w_k, and vice versa. For example,

$$\delta_{jk} = \langle v_j | v_k \rangle = \frac{1}{m_j m_k} \langle M^\dagger w_j^* | M^\dagger w_k^* \rangle = \frac{1}{m_j m_k} \langle w_j | MM^\dagger w_k^* \rangle = \frac{m_k}{m_j} \langle w_j^* | w_k^* \rangle, \tag{D.1.2}$$

which yields $\langle w_k | w_j \rangle = \delta_{jk}$. If M is a real matrix, then the eigenvectors v_k can be chosen to be real, in which case the corresponding w_k are also real.

If v_i is an eigenvector of $M^\dagger M$ with zero eigenvalue, then $0 = v_i^\dagger M^\dagger M v_i = \langle M v_i | M v_i \rangle$, which implies that $M v_i = 0$. Likewise, if w_i^* is an eigenvector of $MM^\dagger$ with zero eigenvalue, then $0 = w_i^{\mathsf{T}} MM^\dagger w_i^* = \langle M^{\mathsf{T}} w_i | M^{\mathsf{T}} w_i \rangle^*$, which implies that $M^{\mathsf{T}} w_i = 0$. Because the eigenvectors of $M^\dagger M$ [$MM^\dagger$] can be chosen orthonormal, the eigenvectors corresponding to the zero eigenvalues of M [$M^\dagger$] can be taken to be orthonormal.[101] Finally, these eigenvectors are also orthogonal to the

[99] One may choose not to work in a basis where the fermion fields are eigenstates of the U(1) charge operator. In this case, all fermions are governed by a complex symmetric mass matrix, which can be Takagi diagonalized according to the procedure described in Appendix D.2.

[100] We define the inner product of two vectors to be $\langle v | w \rangle \equiv v^\dagger w$. Then, v and w are orthonormal if $\langle v | w \rangle = 0$. The norm of a vector is defined by $\| v \| = \langle v | v \rangle^{1/2}$.

[101] This analysis shows that the number of linearly independent zero eigenvectors of $M^\dagger M$ [$MM^\dagger$] with zero eigenvalue, coincides with the number of linearly independent eigenvectors of M [$M^\dagger$] with zero eigenvalue.

eigenvectors corresponding to the non-zero eigenvalues of $M^\dagger M$ [$MM^\dagger$]. That is, if the indices i and j run over the eigenvectors corresponding to the zero and non-zero eigenvalues of $M^\dagger M$ [$MM^\dagger$], respectively, then

$$\langle v_j|v_i\rangle = \frac{1}{m_j}\langle M^\dagger w_j^*|v_i\rangle = \frac{1}{m_j}\langle w_j^*|Mv_i\rangle = 0, \tag{D.1.3}$$

and similarly $\langle w_j|w_i\rangle = 0$.

Thus, we can define the singular values of a general complex $n \times n$ matrix M to be the simultaneous solutions (with real non-negative m_k) of[102]:

$$Mv_k = m_k w_k^*, \qquad w_k^{\mathsf{T}} M = m_k v_k^\dagger. \tag{D.1.4}$$

The corresponding v_k (w_k), normalized to have unit norm, are called the right (left) singular vectors of M. In particular, the number of linearly independent v_k coincides with the number of linearly independent w_k and is equal to n.

Proof of the singular value decomposition theorem. Eqs. (D.1.2) and (D.1.3) imply that the right [left] singular vectors can be chosen to be orthonormal. Consequently, the unitary matrix R [L] can be constructed such that its kth column is given by the right [left] singular vector v_k [w_k]. It then follows from Eq. (D.1.4) that:

$$w_k^{\mathsf{T}} M v_\ell = m_k \delta_{k\ell}, \quad \text{(no sum over } k\text{)}. \tag{D.1.5}$$

In matrix form, Eq. (D.1.5) coincides with Eq. (D.1.1), and the singular value decomposition is established. If M is real, then the right and left singular vectors, v_k and w_k, can be chosen to be real, in which case Eq. (D.1.1) holds for real orthogonal matrices L and R.

The singular values of a complex matrix M are unique (up to ordering), as they correspond to the eigenvalues of $M^\dagger M$ (or equivalently the eigenvalues of $MM^\dagger$). The unitary matrices L and R are not unique. The matrix R must satisfy

$$R^\dagger M^\dagger M R = M_D^2, \tag{D.1.6}$$

which follows directly from Eq. (D.1.1) by computing $M_D^\dagger M_D = M_D^2$. That is, R is a unitary matrix that diagonalizes the non-negative definite matrix $M^\dagger M$. Since the eigenvectors of $M^\dagger M$ are orthonormal, each v_k corresponding to a non-degenerate eigenvalue of $M^\dagger M$ can be multiplied by an arbitrary phase $e^{i\theta_k}$. For the case of degenerate eigenvalues, any orthonormal linear combination of the corresponding eigenvectors is also an eigenvector of $M^\dagger M$. It follows that within the subspace spanned by the eigenvectors corresponding to non-degenerate eigenvalues, R is uniquely determined up to multiplication on the right by an arbitrary diagonal unitary matrix. Within the subspace spanned by the eigenvectors of $M^\dagger M$ corresponding to a degenerate eigenvalue, R is determined up to multiplication on the right by an arbitrary unitary matrix.

Once R is fixed, L is obtained from Eq. (D.1.1):

$$L = (M^{\mathsf{T}})^{-1} R^* M_D. \tag{D.1.7}$$

However, if some of the diagonal elements of M_D are zero, then L is not uniquely defined. Writing M_D in 2×2 block form such that the upper left block is a diagonal matrix with positive diagonal elements and the other three blocks are equal to the zero matrix of the appropriate dimensions, it follows that, $M_D = M_D W$, where

$$W = \left(\begin{array}{c|c} \mathbb{1} & \mathbb{O} \\ \hline \mathbb{O} & W_0 \end{array}\right) \tag{D.1.8}$$

W_0 is an arbitrary unitary matrix whose dimension is equal to the number of zeros that appear in the diagonal elements of M_D, and $\mathbb{1}$ and $\mathbb{O}$ are respectively the identity matrix and zero matrix of the appropriate size. Hence, we can multiply both sides of Eq. (D.1.7) on the right by W, which means that L is only determined up to multiplication on the right by an arbitrary unitary matrix whose form is given by Eq. (D.1.8).[103]

If M is a real matrix, then the derivation of the singular value decomposition of M is given by Eq. (D.1.1), where L and R are real orthogonal matrices. This result is easily established by replacing "phase" with "sign" and replacing "unitary" by "real orthogonal" in the above proof.

[102] One can always find a solution to Eq. (D.1.4) such that the m_k are real and non-negative. Given a solution where m_k is complex, we simply write $m_k = |m_k|e^{i\theta}$ and redefine $w_k \to w_k e^{i\theta}$ to remove the phase θ.

[103] Of course, one can reverse the above procedure by first determining the unitary matrix L. Eq. (D.1.1) implies that $L^{\mathsf{T}} MM^\dagger L^* = M_D^2$, in which case L is determined up to multiplication on the right by an arbitrary [diagonal] unitary matrix within the subspace spanned by the eigenvectors corresponding to the degenerate [non-degenerate] eigenvalues of $MM^\dagger$. Having fixed L, one can obtain $R = M^{-1} L^* M_D$ from Eq. (D.1.1). As above, R is only determined up to multiplication on the right by a unitary matrix whose form is given by Eq. (D.1.8).

D.2. Takagi diagonalization

The mass matrix of neutral fermions (or a system of two-component fermions in a generic basis) is complex and symmetric. This mass matrix must be diagonalized in order to identify the physical fermion mass eigenstates and to compute their masses. However, the fermion mass matrix is *not* diagonalized by the standard unitary similarity transformation. Instead a different diagonalization equation is employed that was discovered by Takagi [111], and rediscovered many times since [147].[104]

Theorem. *For any complex symmetric $n \times n$ matrix M, there exists a unitary matrix Ω such that:*

$$\Omega^{\mathsf{T}} M\, \Omega = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n), \tag{D.2.1}$$

where the m_k are real and non-negative. This is the Takagi diagonalization[105] *of the complex symmetric matrix M.*

In general, the m_k are *not* the eigenvalues of M. Rather, the m_k are the singular values of the symmetric matrix M. From Eq. (D.2.1) it follows that:

$$\Omega^{\dagger} M^{\dagger} M \Omega = M_D^2 = \mathrm{diag}(m_1^2, m_2^2, \ldots, m_n^2). \tag{D.2.2}$$

If all of the singular values m_k are non-degenerate, then one can find a solution to Eq. (D.2.1) for Ω from Eq. (D.2.2). This is no longer true if some of the singular values are degenerate. For example, if $M = \left(\begin{smallmatrix} 0 & m \\ m & 0 \end{smallmatrix}\right)$, then the singular value $|m|$ is doubly degenerate, but Eq. (D.2.2) yields $\Omega^{\dagger}\Omega = \mathbb{1}_{2\times 2}$, which does not specify Ω. That is, in the degenerate case, the physical fermion states *cannot* be determined by the diagonalization of $M^{\dagger}M$. Instead, one must make direct use of Eq. (D.2.1). Below, we shall present a constructive method for determining Ω that is applicable in both the non-degenerate and the degenerate cases.

Eq. (D.2.1) can be rewritten as $M\Omega = \Omega^* M_D$, where the columns of Ω are orthonormal. If we denote the kth column of Ω by v_k, then,

$$M v_k = m_k v_k^*, \tag{D.2.3}$$

where the m_k are the singular values and the vectors v_k are normalized to have unit norm. Following Ref. [261], the v_k are called the *Takagi vectors* of the complex symmetric $n \times n$ matrix M. The Takagi vectors corresponding to non-degenerate non-zero [zero] singular values are unique up to an overall sign [phase]. Any orthogonal [unitary] linear combination of Takagi vectors corresponding to a set of degenerate non-zero [zero] singular values is also a Takagi vector corresponding to the same singular value. Using these results, one can determine the degree of non-uniqueness of the matrix Ω. For definiteness, we fix an ordering of the diagonal elements of M_D.[106] If the singular values of M are distinct, then the matrix Ω is uniquely determined up to multiplication by a diagonal matrix whose entries are either ± 1 (i.e., a diagonal orthogonal matrix). If there are degeneracies corresponding to non-zero singular values, then within the degenerate subspace, Ω is unique up to multiplication on the right by an arbitrary orthogonal matrix. Finally, in the subspace corresponding to zero singular values, Ω is unique up to multiplication on the right by an arbitrary unitary matrix.

For a real symmetric matrix M, the Takagi diagonalization [Eq. (D.2.1)] still holds for a unitary matrix Ω, which is easily determined as follows. Any real symmetric matrix M can be diagonalized by a real orthogonal matrix Z,

$$Z^{\mathsf{T}} M Z = \mathrm{diag}(\varepsilon_1 m_1, \varepsilon_2 m_2, \ldots, \varepsilon_n m_n), \tag{D.2.4}$$

where the m_k are real and non-negative and the $\varepsilon_k m_k$ are the real eigenvalues of M with corresponding signs $\varepsilon_k = \pm 1$.[107] Then, the Takagi diagonalization of M is achieved by taking:

$$\Omega_{ij} = \varepsilon_i^{1/2} Z_{ij}, \quad \text{no sum over } i. \tag{D.2.5}$$

Proof of the Takagi diagonalization. To prove the existence of the Takagi diagonalization of a complex symmetric matrix, it is sufficient to provide an algorithm for constructing the orthonormal Takagi vectors v_k that make up the columns of Ω.

104 Subsequently, it was recognized in Ref. [258] that the Takagi diagonalization was first established for nonsingular complex symmetric matrices by Autonne [259]. In the physics literature, the first proof of Eq. (D.2.1) was given in Ref. [149]. Applications of Takagi diagonalization to the study of neutrino mass matrices can be found in Refs. [5,260].

105 In Ref. [147], Eq. (D.2.1) is called the Takagi factorization of a complex symmetric matrix. We choose to refer to this as Takagi *diagonalization* to emphasize and contrast this with the more standard diagonalization of normal matrices by a unitary similarity transformation. In particular, not all *complex* symmetric matrices are diagonalizable by a similarity transformation, whereas complex symmetric matrices are *always* Takagi diagonalizable.

106 Permuting the order of the singular values is equivalent to permuting the order of the columns of Ω.

107 In the case of $m_k = 0$, we conventionally choose the corresponding $\varepsilon_k = +1$.

This is achieved by rewriting the $n \times n$ complex matrix equation $Mv = mv^*$ [with m real and non-negative] as a $2n \times 2n$ real matrix equation [262,263]:

$$M_R \begin{pmatrix} \mathrm{Re}\, v \\ \mathrm{Im}\, v \end{pmatrix} \equiv \begin{pmatrix} \mathrm{Re}\, M & -\mathrm{Im}\, M \\ -\mathrm{Im}\, M & -\mathrm{Re}\, M \end{pmatrix} \begin{pmatrix} \mathrm{Re}\, v \\ \mathrm{Im}\, v \end{pmatrix} = m \begin{pmatrix} \mathrm{Re}\, v \\ \mathrm{Im}\, v \end{pmatrix}, \quad \text{where } m \geq 0. \tag{D.2.6}$$

Since $M = M^{\mathsf{T}}$, the $2n \times 2n$ matrix $M_R \equiv \left(\begin{smallmatrix} \mathrm{Re}\, M & -\mathrm{Im}\, M \\ -\mathrm{Im}\, M & -\mathrm{Re}\, M \end{smallmatrix}\right)$is a real symmetric matrix.[108] In particular, M_R is diagonalizable by a real orthogonal similarity transformation, and its eigenvalues are real. Moreover, if m is an eigenvalue of M_R with eigenvector $(\mathrm{Re}\, v, \mathrm{Im}\, v)$, then $-m$ is an eigenvalue of M_R with (orthogonal) eigenvector $(-\mathrm{Im}\, v, \mathrm{Re}\, v)$. This observation implies that M_R has an equal number of positive and negative eigenvalues and an even number of zero eigenvalues.[109] Thus, Eq. (D.2.3) has been converted into an ordinary eigenvalue problem for a real symmetric matrix. Since $m \geq 0$, we solve the eigenvalue problem $M_R u = mu$ for the real eigenvectors $u \equiv (\mathrm{Re}\, v, \mathrm{Im}\, v)$ corresponding to the non-negative eigenvalues of M_R,[110] which then immediately yields the complex Takagi vectors, v. It is straightforward to prove that the total number of linearly independent Takagi vectors is equal to n. Simply note that the orthogonality of $(\mathrm{Re}\, v_1, \mathrm{Im}\, v_1)$ and $(-\mathrm{Im}\, v_1, \mathrm{Re}\, v_1)$ with $(\mathrm{Re}\, v_2, \mathrm{Im}\, v_2)$ implies that $v_1^\dagger v_2 = 0$.

Thus, we have derived a constructive method for obtaining the Takagi vectors v_k. If there are degeneracies, one can always choose the v_k in the degenerate subspace to be orthonormal. The Takagi vectors then make up the columns of the matrix Ω in Eq. (D.2.1). A numerical package for performing the Takagi diagonalization of a complex symmetric matrix has recently been presented in Ref. [264] (see also Refs. [261,265] for previous numerical approaches to Takagi diagonalization).

D.3. Relation between Takagi diagonalization and singular value decomposition

The Takagi diagonalization is a special case of the singular value decomposition. If the complex matrix M in Eq. (D.1.1) is symmetric, $M = M^{\mathsf{T}}$, then the Takagi diagonalization corresponds to $\Omega = L = R$. In this case, the right and left singular vectors coincide ($v_k = w_k$) and are identified with the Takagi vectors defined in Eq. (D.2.3). However as previously noted, the matrix Ω cannot be determined from Eq. (D.2.2) in cases where there is a degeneracy among the singular values.[111] For example, one possible singular value decomposition of the matrix $M = \left(\begin{smallmatrix} 0 & m \\ m & 0 \end{smallmatrix}\right)$ [with m assumed real and positive] can be obtained by choosing $R = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ and $L = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, in which case $L^{\mathsf{T}} M R = \left(\begin{smallmatrix} m & 0 \\ 0 & m \end{smallmatrix}\right) = M_D$. Of course, this is not a Takagi diagonalization because $L \neq R$. Since R is only defined modulo the multiplication on the right by an arbitrary 2×2 unitary matrix $\mathcal{O}$, then at least one singular value decomposition exists that is also a Takagi diagonalization. For the example under consideration, it is not difficult to deduce the Takagi diagonalization: $\Omega^{\mathsf{T}} M \Omega = M_D$, where

$$\Omega = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \mathcal{O}, \tag{D.3.1}$$

and $\mathcal{O}$ is any 2×2 orthogonal matrix.

Since the Takagi diagonalization is a special case of the singular value decomposition, it seems plausible that one can prove the former from the latter. This turns out to be correct; for completeness, we provide the proof below. Our second proof depends on the following lemma:

Lemma. *For any symmetric unitary matrix V, there exists a unitary matrix U such that $V = U^{\mathsf{T}} U$.*

Proof of the Lemma: For any $n \times n$ unitary matrix V, there exists an hermitian matrix H such that $V = \exp(iH)$ (this is the polar decomposition of V). If $V = V^{\mathsf{T}}$ then $H = H^{\mathsf{T}} = H^*$ (since H is hermitian); therefore H is real symmetric. But, any real symmetric matrix can be diagonalized by an orthogonal transformation. It follows that V can also be diagonalized by an orthogonal transformation. Since the eigenvalues of any unitary matrix are pure phases, there exists a real orthogonal matrix Q such that $Q^{\mathsf{T}} V Q = \mathrm{diag}\,(e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_n})$. Thus, the unitary matrix,

$$U = \mathrm{diag}\,(e^{i\theta_1/2}, e^{i\theta_2/2}, \ldots, e^{i\theta_n/2})\, Q^{\mathsf{T}}, \tag{D.3.2}$$

satisfies $V = U^{\mathsf{T}} U$ and the lemma is proved. Note that U is unique modulo multiplication on the left by an arbitrary real orthogonal matrix.

108 The $2n \times 2n$ matrix M_R is a real representation of the $n \times n$ complex matrix M.

109 Note that $(-\mathrm{Im}\, v, \mathrm{Re}\, v)$ corresponds to replacing v_k in Eq. (D.2.3) by iv_k. However, for $m < 0$ these solutions are not relevant for Takagi diagonalization (where the m_k are by definition non-negative). The case of $m = 0$ is considered in footnote 110.

110 For $m = 0$, the corresponding vectors $(\mathrm{Re}\, v, \mathrm{Im}\, v)$ and $(-\mathrm{Im}\, v, \mathrm{Re}\, v)$ are two linearly independent eigenvectors of M_R; but these yield only one independent Takagi vector v (since v and iv are linearly dependent).

111 This is in contrast to the singular value decomposition, where R can be determined from Eq. (D.1.6) modulo right multiplication by a [diagonal] unitary matrix in the [non-]degenerate subspace and L is then determined by Eq. (D.1.7) modulo multiplication on the right by Eq. (D.1.8).

Second Proof of the Takagi diagonalization. Starting from the singular value decomposition of M, there exist unitary matrices L and R such that $M = L^* M_D R^\dagger$, where M_D is the diagonal matrix of singular values. Since $M = M^\mathsf{T} = R^* M_D L^\dagger$, we have two different singular value decompositions for M. However, as noted below Eq. (D.1.6), R is unique modulo multiplication on the right by an arbitrary [diagonal] unitary matrix, V, within the [non-]degenerate subspace. Thus, it follows that a [diagonal] unitary matrix V exists such that $L = RV$. Moreover, $V = V^\mathsf{T}$. This is manifestly true within the non-degenerate subspace where V is diagonal. Within the degenerate subspace, M_D is proportional to the identity matrix so that $L^* R^\dagger = R^* L^\dagger$. Inserting $L = RV$ then yields $V^\mathsf{T} = V$. Using the lemma proved above, there exists a unitary matrix U such that $V = U^\mathsf{T} U$. That is,

$$L = RU^\mathsf{T} U, \tag{D.3.3}$$

for some unitary matrix U. Moreover, it is now straightforward to show that

$$M_D U^* = U^* M_D. \tag{D.3.4}$$

To see this, note that within the degenerate subspace, Eq. (D.3.4) is trivially true since M_D is proportional to the identity matrix. Within the non-degenerate subspace V is diagonal; hence we may choose $U = U^\mathsf{T} = V^{1/2}$, so that Eq. (D.3.4) is true since diagonal matrices commute. Using Eqs. (D.3.3) and (D.3.4), we can write the singular value decomposition of M as follows

$$M = L^* M_D R^\dagger = R^* U^\dagger U^* M_D R^\dagger = (RU^\mathsf{T})^* M_D U^* R^\dagger = \Omega^* M_D \Omega^\dagger, \tag{D.3.5}$$

where $\Omega \equiv RU^\mathsf{T}$ is a unitary matrix. Thus the existence of the Takagi diagonalization of an arbitrary complex symmetric matrix [Eq. (D.2.1)] is once again proved.

In the diagonalization of the two-component fermion mass matrix, M, the eigenvalues of $M^\dagger M$ typically fall into two classes—non-degenerate eigenvalues corresponding to neutral fermion mass eigenstates and degenerate pairs corresponding to charged (Dirac) mass eigenstates. In this case, the sector of the neutral fermions corresponds to a non-degenerate subspace of the space of fermion fields. Hence, in order to identify the neutral fermion mass eigenstates, it is sufficient to diagonalize $M^\dagger M$ with a unitary matrix R [as in Eq. (D.1.6)], and then adjust the overall phase of each column of R so that the resulting matrix Ω satisfies $\Omega^\mathsf{T} M \Omega = M_D$, where M_D is a diagonal matrix of the non-negative fermion masses. This last result is a consequence of Eqs. (D.3.3)–(D.3.5), where $\Omega = RV^{1/2}$ and V is a diagonal matrix of phases.

D.4. Reduction of a complex antisymmetric matrix to the real normal form

In the case of two-component fermions that transform under a pseudo-real representation of a compact Lie group [cf. Eq. (3.2.35)], the corresponding mass matrix is in general complex and antisymmetric. In this case, one needs the antisymmetric analogue of the Takagi diagonalization of a complex symmetric matrix [147].

Theorem. *For any complex [or real] antisymmetric $n \times n$ matrix M, there exists a unitary [or real orthogonal] matrix U such that:*

$$U^\mathsf{T} M U = N \equiv \text{diag}\left\{ \begin{pmatrix} 0 & m_1 \\ -m_1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & m_2 \\ -m_2 & 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 & m_p \\ -m_p & 0 \end{pmatrix}, \mathbb{O}_{n-2p} \right\}, \tag{D.4.1}$$

where N is written in block diagonal form with 2×2 matrices appearing along the diagonal, followed by an $(n-2p) \times (n-2p)$ block of zeros (denoted by $\mathbb{O}_{n-2p}$), and the m_j are real and positive. N is called the real normal form of an antisymmetric matrix [149,266,267].

Proof. A number of proofs can be found in the literature [148,149,266–268]. Here we provide a proof inspired by Ref. [266]. Following Appendix D.1, we first consider the eigenvalue equation for $M^\dagger M$:

$$M^\dagger M v_k = m_k^2 v_k, \quad m_k > 0, \quad \text{and} \quad M^\dagger M u_k = 0, \tag{D.4.2}$$

where we have distinguished the eigenvectors corresponding to positive eigenvalues and zero eigenvalues, respectively. The quantities m_k are the positive singular values of M. Noting that $u_k^\dagger M^\dagger M u_k = \langle M u_k \,|\, M u_k \rangle = 0$, it follows that

$$M u_k = 0, \tag{D.4.3}$$

so that the u_k are the eigenvectors corresponding to the zero eigenvalues of M. For each eigenvector of $M^\dagger M$ with $m_k \neq 0$, we define a new vector

$$w_k \equiv \frac{1}{m_k} M^* v_k^*. \tag{D.4.4}$$

It follows that $m_k^2 v_k = M^\dagger M v_k = m_k M^\dagger w_k^*$, which yields $M^\dagger w_k^* = m_k v_k$. Comparing with Eq. (D.1.4), we identify v_k and w_k as the right and left singular vectors, respectively, corresponding to the non-zero singular values of M. For any antisymmetric matrix, $M^\dagger = -M^*$. Hence,

$$M v_k = m_k w_k^*, \qquad M w_k = -m_k v_k^*, \tag{D.4.5}$$

and

$$M^\dagger M w_k = -m_k M^\dagger v_k^* = m_k M^* v_k^* = m_k^2 w_k, \quad m_k > 0. \tag{D.4.6}$$

That is, the w_k are also eigenvectors of $M^\dagger M$.

The key observation is that for fixed k the vectors v_k and w_k are orthogonal, since Eq. (D.4.5) implies that:

$$\langle w_k|v_k\rangle = \langle v_k|w_k\rangle^* = -\frac{1}{m_k^2}\langle Mw_k|Mv_k\rangle = -\frac{1}{m_k^2}\langle w_k|M^\dagger M v_k\rangle = -\langle w_k|v_k\rangle\,, \tag{D.4.7}$$

which yields $\langle w_k|v_k\rangle = 0$. Thus, if all the m_k are distinct, it follows that m_k^2 is a doubly degenerate eigenvalue of $M^\dagger M$, with corresponding linearly independent eigenvectors v_k and w_k, where $k = 1, 2, \ldots, p$ (and $p \le \frac{1}{2}n$). The remaining zero eigenvalues are $(n-2p)$-fold degenerate, with corresponding eigenvectors u_k (for $k = 1, 2, \ldots, n-2p$). If some of the m_k are degenerate, these conclusions still apply. For example, suppose that $m_j = m_k$ for $j \neq k$, which means that m_k^2 is at least a three-fold degenerate eigenvalue of $M^\dagger M$. Then, there must exist an eigenvector v_j that is orthogonal to v_k and w_k such that $M^\dagger M v_j = m_k^2 v_j$. We now construct $w_j \equiv M^* v_j^*/m_k$ according to Eq. (D.4.4). According to Eq. (D.4.7), w_j is orthogonal to v_j. But, we still must show that w_j is also orthogonal to v_k and w_k. But this is straightforward:

$$\langle w_j|w_k\rangle = \langle w_k|w_j\rangle^* = \frac{1}{m_k^2}\langle Mv_k|Mv_j\rangle = \frac{1}{m_k^2}\langle v_k|M^\dagger M v_j\rangle = \langle v_k|v_j\rangle = 0, \tag{D.4.8}$$

$$\langle w_j|v_k\rangle = \langle v_k|w_j\rangle^* = -\frac{1}{m_k^2}\langle Mw_k|Mv_j\rangle = -\frac{1}{m_k^2}\langle w_k|M^\dagger M v_j\rangle = -\langle w_k|v_j\rangle = 0, \tag{D.4.9}$$

where we have used the assumed orthogonality of v_j with v_k and w_k, respectively. If follows that v_j, w_j, v_k and w_k are linearly independent eigenvectors corresponding to a four-fold degenerate eigenvalue m_k^2 of $M^\dagger M$. Additional degeneracies are treated in the same way.

Thus, the number of non-zero eigenvalues of $M^\dagger M$ must be an even number, denoted by $2p$ above. Moreover, one can always choose the complete set of eigenvectors $\{u_k, v_k, w_k\}$ of $M^\dagger M$ to be orthonormal. These orthonormal vectors can be used to construct a unitary matrix U with matrix elements:

$$\begin{aligned} &U_{\ell,2k-1} = (w_k)_\ell, \qquad U_{\ell,2k} = (v_k)_\ell, \quad k = 1, 2, \ldots, p, \\ &U_{\ell,k+2p} = (u_k)_\ell, \quad k = 1, 2, \ldots, n-2p, \end{aligned} \tag{D.4.10}$$

for $\ell = 1, 2, \ldots, n$, where e.g., $(v_k)_\ell$ is the ℓth component of the vector v_k with respect to the standard orthonormal basis. The orthonormality of $\{u_k, v_k, w_k\}$ implies that $(U^\dagger U)_{\ell k} = \delta_{\ell k}$ as required. Eqs. (D.4.3) and (D.4.5) are thus equivalent to the matrix equation $MU = U^* N$, which immediately yields Eq. (D.4.1), and the theorem is proven. If M is a real antisymmetric matrix, then all the eigenvectors of $M^\dagger M$ can be chosen to be real, in which case U is a real orthogonal matrix.

Finally, we address the non-uniqueness of the matrix U. For definiteness, we fix an ordering of the 2×2 blocks containing the m_k in the matrix N. In the subspace corresponding to a non-zero singular value of degeneracy d, U is unique up to multiplication on the right by a $2d \times 2d$ unitary matrix S that satisfies:

$$S^{\mathsf{T}} J S = J, \tag{D.4.11}$$

where the $2d \times 2d$ matrix J, defined by

$$J = \mathrm{diag}\left\{\begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}, \ldots, \begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}\right\}, \tag{D.4.12}$$

is a block diagonal matrix with d blocks of 2×2 matrices. A unitary matrix S that satisfies Eq. (D.4.11) is an element of the unitary symplectic group, $\mathrm{Sp}(d)$. If there are no degeneracies among the m_k, then $d = 1$. Identifying $\mathrm{Sp}(1) \cong \mathrm{SU}(2)$, it follows that within the subspace corresponding to a non-degenerate singular value, U is unique up to multiplication on the right by an arbitrary SU(2) matrix. Finally, in the subspace corresponding to the zero eigenvalues of M, U is unique up to multiplication on the right by an arbitrary unitary matrix.

Appendix E. Lie group theoretical techniques for gauge theories

E.1. Basic facts about Lie groups, Lie algebras and their representations

Consider a compact connected Lie Group G [269]. The most general form for G is a direct product of compact simple groups and U(1) groups. If no U(1) factors are present, then G is semisimple. For any $U \in G$,

$$U = \exp(-i\theta^a \boldsymbol{T^a}), \tag{E.1.1}$$

where the $\boldsymbol{T^a}$ are called the generators of G, and the θ^a are real numbers that parameterize the elements of G. The corresponding real Lie algebra $\mathfrak{g}$ consists of arbitrary real linear combinations of the generators, $\theta^a \boldsymbol{T^a}$. The Lie group generators $\boldsymbol{T^a}$ satisfy the commutation relations:

$$[\boldsymbol{T^a}, \boldsymbol{T^b}] = i f_c^{ab} \boldsymbol{T^c}, \tag{E.1.2}$$

where the real structure constants f_c^{ab} define the compact Lie algebra. The generator indices run over $a, b, c = 1, 2, \ldots, d_G$, where d_G is the dimension of the Lie algebra. For compact Lie algebras, the Killing form $g^{ab} = \mathrm{Tr}(\boldsymbol{T^a T^b})$ is positive definite, so one can always choose a basis for the Lie algebra in which $g^{ab} \propto \delta^{ab}$ (where the proportionality constant is a positive real number). With respect to this new basis, the structure constants $f^{abc} \equiv g^{ad} f_d^{bc}$ are totally antisymmetric with respect to the interchange of the indices a, b and c. Henceforth, we shall always assume that such a *preferred* basis of generators has been chosen.

The elements of the compact Lie group G act on a multiplet of fields that transform under some d_R-dimensional representation R of G. The group elements $U \in G$ are represented by $d_R \times d_R$ unitary matrices, $D_R(U) = \exp(-i\theta^a \boldsymbol{T^a_R})$, where the $\boldsymbol{T^a_R}$ are $d_R \times d_R$ hermitian matrices that satisfy Eq. (E.1.2) and thus provide a representation of the Lie group generators. For any representation R of a semisimple group, $\mathrm{Tr}\, \boldsymbol{T^a_R} = 0$ for all a. A representation R' is unitarily equivalent to R if there exists a fixed unitary matrix S such that $D_{R'}(U) = S^{-1} D_R(U) S$ for all $U \in G$. Similarly, the corresponding generators satisfy $\boldsymbol{T^a_{R'}} = S^{-1} \boldsymbol{T^a_R} S$ for all $a = 1, 2, \ldots, d_G$.

For compact semisimple Lie groups, two representations are noteworthy. If G is one of the classical groups, SU(N) [for $N \geq 2$], SO(N) [for $N \geq 3$] or Sp($N/2$) [the latter is defined by Eqs. (D.4.11) and (D.4.12) for even $N \geq 2$], then the $N \times N$ matrices that define these groups comprise the *fundamental (or defining) representation* F, with $d_F = N$. For example, the fundamental representation of SU(N) consists of $N \times N$ unitary matrices with determinant equal to one, and the corresponding generators comprise a suitably chosen basis for the $N \times N$ traceless hermitian matrices. Every Lie group G also possesses an *adjoint representation* A, with $d_A = d_G$. The matrix elements of the generators in the adjoint representation are given by[112]

$$(\boldsymbol{T^a_A})^{bc} = -i f^{abc}. \tag{E.1.3}$$

Given the unitary representation matrices $D_R(U)$ of the representation R of G, the matrices $[D_R(U)]^*$ constitute the *conjugate* representation R^*. Equivalently, if the $\boldsymbol{T^a_R}$ comprise a representation of the Lie algebra $\mathfrak{g}$, then the $-(\boldsymbol{T^a_R})^* = -(\boldsymbol{T^a_R})^{\mathsf{T}}$ comprise a representation R^* of $\mathfrak{g}$ of the same dimension d_R. If R and R^* are unitarily equivalent representations, then we say that the representation R is *self-conjugate*. Otherwise, we say that the representation R is *complex*, or "strictly complex" in the language of Ref. [270]. However, the representation matrices $D_R(U)$ of a self-conjugate representation can also be complex. We can then define two classes of self-conjugate representations. If R and R^* are unitarily equivalent to a representation R' that satisfies the reality property $[D_{R'}(U)]^* = [D_{R'}(U)]$ for all $U \in G$ (equivalently, the matrices $i\boldsymbol{T^a_{R'}}$ are real for all a), then R is said to be *real*, or "strictly real" in the language of Ref. [270]. If R and R^* are unitarily equivalent representations, but neither is unitarily equivalent to a representation that satisfies the reality property above, then R is said to be *pseudo-real*.

Henceforth, we drop the adjective "strictly" and simply refer to real, pseudo-real and complex representations. Self-conjugate representations are either real or pseudo-real. An important theorem states that for self-conjugate representations, there exists a constant unitary matrix W such that [270]

$$[D_R(U)]^* = W D_R(U) W^{-1}, \quad \text{or equivalently, } (i\boldsymbol{T^a_R})^* = W(i\boldsymbol{T^a_R})W^{-1}, \tag{E.1.4}$$

where

$$WW^* = \mathbb{1}, \qquad W^{\mathsf{T}} = W, \qquad \text{for real representations}, \tag{E.1.5}$$

$$WW^* = -\mathbb{1}, \qquad W^{\mathsf{T}} = -W, \qquad \text{for pseudo-real representations}, \tag{E.1.6}$$

and $\mathbb{1}$ is the $d_R \times d_R$ identity matrix. Taking the determinant of Eq. (E.1.6), and using the fact that W is unitary (and hence invertible), it follows that $1 = (-1)^{d_R}$. Therefore, a pseudo-real representation must be even-dimensional.

If we redefine the basis for the Lie group generators by $\boldsymbol{T^a_R} \to V^{-1} \boldsymbol{T^a_R} V$, where V is unitary, then $W \to V^{\mathsf{T}} W V$. We can make use of this change of basis to transform W to a canonical form. Since W is unitary, its singular values (i.e. the positive square roots of the eigenvalues of $W^\dagger W$) are all equal to 1. Hence, in the two cases corresponding to $W^{\mathsf{T}} = \pm W$, respectively, Eqs. (D.2.1) and (D.4.1) yield the following canonical forms (for an appropriately chosen V),

$$W = \mathbb{1}, \quad \text{for a real representation } R, \text{ with } \varepsilon_\eta = +1, \tag{E.1.7}$$

$$W = J, \quad \text{for a pseudo-real representation } R, \text{ with } \varepsilon_\eta = -1, \tag{E.1.8}$$

where $J \equiv \mathrm{diag}\left\{ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\}$ is a $d_R \times d_R$ matrix (and d_R is even).

112 Since the f^{abc} are real, the $i\boldsymbol{T^a_A}$ are real antisymmetric matrices. The heights of the adjoint labels a, b and c are not significant, as they can be lowered by the inverse Killing form given by $g_{ab} \propto \delta_{ab}$ in the preferred basis.

There are many examples of complex, real and pseudo-real representations in mathematical physics. For example, the fundamental representation of SU(N) is complex for $N \geq 3$. The adjoint representation of any compact Lie group is real [cf. footnote 112]. The simplest example of a pseudo-real representation is the two-dimensional representation of SU(2),[113] where $\boldsymbol{T^a} = \frac{1}{2}\tau^a$ (and the τ^a are the usual Pauli matrices). More generally, the generators of a pseudo-real representation must satisfy

$$(i\boldsymbol{T^a_R})^* = C^{-1}(i\boldsymbol{T^a_R})C, \tag{E.1.9}$$

for some fixed unitary antisymmetric matrix C [previously denoted by W^{-1} in Eqs. (E.1.4) and (E.1.6)]. For the doublet representation of SU(2) just given, $C^{ab} = (i\tau^2)^{ab} \equiv \epsilon^{ab}$ is the familiar SU(2)-invariant tensor.

Finally, we note that for U(1), all irreducible representations are one-dimensional. The structure constants vanish and any d-dimensional representation of the U(1)-generator is given by the $d \times d$ identity matrix multiplied by the corresponding U(1)-charge. For a Lie group that is a direct product of a semisimple group and U(1) groups, $\mathrm{Tr}\,\boldsymbol{T^a_R}$ is non-zero when a corresponds to one of the U(1)-generators, unless the sum of the corresponding U(1)-charges of the states of the representation R vanishes.

E.2. The quadratic and cubic index and Casimir operator

In this section, we define the index and Casimir operator of a representation of a compact semisimple Lie algebra $\mathfrak{g}$. The *index* $I_2(R)$ of the representation R is defined by [269,271–273]

$$\mathrm{Tr}(\boldsymbol{T^a_R T^b_R}) = I_2(R)\delta^{ab}, \tag{E.2.1}$$

where $I_2(R)$ is a positive real number that depends on R. Once $I_2(R)$ is defined for one representation, its value is uniquely fixed for any other representation. In the case of a simple compact Lie algebra $\mathfrak{g}$, it is traditional to normalize the generators of the fundamental (or defining) representation F according to[114]

$$\mathrm{Tr}(\boldsymbol{T^a_F T^b_F}) = \tfrac{1}{2}\delta^{ab}. \tag{E.2.2}$$

If the representation R is reducible, it can be decomposed into the direct sum of irreducible representations, $R = \sum_k R_k$. In this case, the index of R is given by

$$I_2(R) = \sum_k I_2(R_k). \tag{E.2.3}$$

The index of a tensor product of two representations R_1 and R_2 is given by [271]

$$I_2(R_1 \otimes R_2) = d_{R_1} I_2(R_2) + d_{R_2} I_2(R_1). \tag{E.2.4}$$

Finally, we note that if R^* is the complex conjugate of the representation R, then

$$I_2(R^*) = I_2(R). \tag{E.2.5}$$

A Casimir operator of a Lie algebra $\mathfrak{g}$ is an operator that commutes with all the generators $\boldsymbol{T^a}$. If the representation of the $\boldsymbol{T^a}$ is *irreducible*, then Schur's lemma implies that the Casimir operator is a multiple of the identity. The proportionality constant depends on the representation R. The quadratic Casimir operator of an *irreducible* representation R is given by

$$(\boldsymbol{T^2_R})_i{}^j \equiv (\boldsymbol{T^a_R})_i{}^k (\boldsymbol{T^a_R})_k{}^j = C_R \delta_i{}^j, \tag{E.2.6}$$

where the sum over the repeated indices are implicit and $i, j, k = 1, 2 \ldots d_R$. A simple computation then yields the eigenvalue of the quadratic Casimir operator, C_R,

$$C_R = \frac{I_2(R) d_G}{d_R}. \tag{E.2.7}$$

For a simple Lie algebra (where the adjoint representation is irreducible), it immediately follows that $C_A = I_2(A)$. For a reducible representation, $\boldsymbol{T^2}$ is a block diagonal matrix consisting of $d_{R_k} \times d_{R_k}$ blocks given by $C_{R_k}\mathbb{1}$ for each irreducible component R_k of R.

The example of the simple Lie algebra $\mathfrak{su}(N)$ is well known. The dimension of this Lie algebra (equal to the number of generators) is given by $N^2 - 1$. As previously noted, $d_F = N$ and $I_2(F) = \frac{1}{2}$. It then follows that $C_F = (N^2 - 1)/(2N)$. One can also check that $C_A = I_2(A) = N$.

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113 No unitary matrix W exists such that the $Wi\tau^a W^{-1}$ are real for all $a = 1, 2, 3$. Thus, the two-dimensional representation of SU(2) is not real. However, $(i\tau^a)^* = (i\tau^2)(i\tau^a)(i\tau^2)^{-1}$ for $a = 1, 2, 3$, which proves that the two-dimensional representation of SU(2) is pseudo-real.

114 In the literature, the index is often defined as the ratio $I_2(R)/I_2(F)$, where $I_2(F)$ is fixed by some convention. This has the advantage that the index of R is independent of the normalization convention of the generators. In this Appendix, we will simply refer to $I_2(R)$ as the index.

The Lie algebras $\mathfrak{su}(N)$ $[N \geq 3]$ are the only simple Lie algebra that possesses a cubic Casimir operator. First, we define the symmetrized trace of three generators [273,274]:

$$D^{abc} \equiv \text{Str}\,(\boldsymbol{T^a T^b T^c}) = \frac{1}{6}\text{Tr}(\boldsymbol{T^a T^b T^c} + \text{perm.}), \tag{E.2.8}$$

where "perm." indicates five other terms obtained by permuting the indices a, b and c in all possible ways. Due to the properties of the trace, it follows that for a given representation R,

$$D^{abc}(R) = \tfrac{1}{2}\text{Tr}\left[\{\boldsymbol{T^a_R}, \boldsymbol{T^b_R}\}\boldsymbol{T^c_R}\right]. \tag{E.2.9}$$

For the N-dimensional defining representation of $\mathfrak{su}(N)$, it is conventional to define

$$d^{abc} \equiv 2\text{Tr}\left[\{\boldsymbol{T^a_F}, \boldsymbol{T^b_F}\}\boldsymbol{T^c_F}\right]. \tag{E.2.10}$$

One important property of the d^{abc} is [275,276]:

$$d^{abc}d^{abc} = \frac{(N^2-1)(N^2-4)}{N}. \tag{E.2.11}$$

In general, $D^{abc}(R)$ is proportional to d^{abc}. In particular, the *cubic index* $I_3(R)$ of a representation R is defined such that [273,275,277],

$$D^{abc}(R) = I_3(R)d^{abc}. \tag{E.2.12}$$

Having fixed $I_3(F) = \frac{1}{4}$, the cubic index is uniquely determined for all representations of $\mathfrak{su}(N)$ [275,277–279]. As in the case of the quadratic index $I_2(R)$, we have:

$$I_3(R) = \sum_k I_3(R_k), \tag{E.2.13}$$

for a reducible representation $R = \sum_k R_k$. The cubic index of a tensor product of two representations R_1 and R_2 is given by [277]

$$I_3(R_1 \otimes R_2) = d_{R_1}I_3(R_2) + d_{R_2}I_3(R_1). \tag{E.2.14}$$

If the generators of the representation R are $\boldsymbol{T^a_R}$, then the generators of the complex conjugate representation R^* are $-\boldsymbol{T^a_R}^{\mathsf{T}}$. It then follows that

$$I_3(R^*) = -I_3(R). \tag{E.2.15}$$

In particular, the cubic index of a self-conjugate representation vanishes. Note that the converse is not true. That is, it is possible for the cubic index of a complex representation of $\mathfrak{su}(N)$ to vanish in special circumstances [279].

One can show that among the simple Lie groups, $D^{abc} = 0$ except for the case of SU(N), when $N \geq 3$ [275]. For any non-semisimple Lie group (i.e., a Lie group that is a direct product of simple Lie groups and at least one U(1) factor), D^{abc} is generally non-vanishing. For example, suppose that the $\boldsymbol{T^a_R}$ constitute an irreducible representation of the generators of $G\times$U(1), where G is a semisimple Lie group. Then the U(1) generator (which we denote by setting $\boldsymbol{a} = \boldsymbol{Q}$) is $\boldsymbol{T^Q_R} \equiv q\mathbb{1}$, where q is the corresponding U(1)-charge. It then follows that $D^{Qab} = qI_2(R)\delta^{ab}$. More generally, for a compact non-semisimple Lie group, D^{abc} can be non-zero when either one or three of its indices corresponds to a U(1) generator.

In the computation of the anomaly [cf. Section 6.26], the quantity $\text{Tr}(\boldsymbol{T^a_R T^b_R T^c_R})$ appears. We can evaluate this trace using Eqs. (E.1.2) and (E.2.12):

$$\text{Tr}(\boldsymbol{T^a_R T^b_R T^c_R}) = I_3(R)d^{abc} + \frac{i}{2}I_2(R)f^{abc}. \tag{E.2.16}$$

The cubic Casimir operator of an *irreducible* representation R is given by

$$(\boldsymbol{T^3_R})_i{}^j \equiv d^{abc}(\boldsymbol{T^a_R T^b_R T^c_R})_i{}^j = C_{3R}\delta_i{}^j. \tag{E.2.17}$$

Using Eqs. (E.2.11) and (E.2.12), we obtain a relation between the eigenvalue of the cubic Casimir operator, C_{3R} and the cubic index [275]:

$$C_{3R} = \frac{(N^2-1)(N^2-4)I_3(R)}{Nd_R}. \tag{E.2.18}$$

Again, we provide two examples. For the fundamental representation of $\mathfrak{su}(N)$, $I_3(F) = \frac{1}{4}$ and $C_{3F} = (N^2-1)(N^2-4)/(4N^2)$. For the adjoint representation, $I_3(A) = C_{3A} = 0$, since the adjoint representation is self-conjugate. A general formula for the eigenvalue of the cubic Casimir operator in an arbitrary $\mathfrak{su}(N)$ representation [or equivalently the cubic index $I_3(R)$, which is related to C_{3R} by Eq. (E.2.18)] can be found in Refs. [275,277–279].